Entanglement in Quantum Spin Chains, Symmetry Classes of Random Matrices, and Conformal Field Theory

J.P. Keating[1] and F. Mezzadri[1]

[1] *School of Mathematics, University of Bristol, Bristol BS8 1TW, UK.*

We compute the entropy of entanglement between the first N spins and the rest of the system in the ground states of a general class of quantum spin-chains. We show that under certain conditions the entropy can be expressed in terms of averages over ensembles of random matrices. These averages can be evaluated, allowing us to prove that at critical points the entropy grows like $\kappa \log_2 N + \tilde{\kappa}$ as $N \to \infty$, where κ and $\tilde{\kappa}$ are determined explicitly. In an important class of systems, κ is equal to one-third of the central charge of an associated Virasoro algebra. Our expression for κ therefore provides an explicit formula for the central charge.

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Entanglement has recently come to be viewed as an important physical resource for manipulating quantum information. The problem of quantifying it is, however, still poorly understood, especially when the entanglement is shared between more than two systems. When the entanglement of a pure state is shared between two parties, i.e. in a *bipartite system*, Bennett *et al* [1] have shown that it is consistent to define it as the von Neumann entropy of either of the two parts. We consider here the general class of quantum spin chains arising from quadratic chains of fermionic operators in their ground state. These systems are partitioned into two contiguous subchains. If the ground state is non-degenerate, this subdivision creates a pure bipartite system; our main result is to calculate its entanglement entropy by relating the problem to one in random matrix theory.

As is well known, the systems we are studying exhibit quantum phase transitions. These manifest themselves as qualitative changes in the decay of correlations: algebraic at a critical point and exponential decay away from it. Entanglement plays a fundamental role in the quantum phase transitions that occur in interacting lattice systems at zero temperature [2, 3, 4, 5, 6, 7, 8]. Under these conditions the system is in the ground state, which is also a pure state, and any correlations must be a consequence of the fact the ground state is entangled. It follows immediately that the entanglement changes qualitatively at critical points.

In this context, Vidal *et al.* [3] studied the ground states of a wide range of one-dimensional spin models partitioned into two consecutive subchains. They observed numerically that, when the Hamiltonian undergoes a phase transition, the entanglement of formation of these bipartite systems grows logarithmically with the size N of one of the two parts. Jin and Korepin [4] then proved that the entropy grows like $\frac{1}{3}\log_2 N$ in the XX model, for which the Hamiltonian is

$$H_\alpha = -\frac{\alpha}{2}\sum_{j=0}^{M-1}\left[\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right] - \sum_{j=0}^{M-1}\sigma_j^z, \qquad (1)$$

where σ^a denotes the Pauli matrices and $a = x, y, z$. Recently, Korepin [5] and Calabrese and Cardy [6] showed, using conformal field-theoretic arguments developed by Holzhey *et al.* [9], that the logarithmic divergence of the entanglement in one dimensional systems is a general consequence of the logarithmic growth of the entropy with the size of the system at phase transitions. These arguments determine the constant multiplying the leading order $\log_2 N$ term in the asymptotics to be one-third of the central charge of the associated Virasoro algebra [10].

We show here that if a quantum spin-chain Hamiltonian posses certain symmetries, the entanglement can be expressed as an average over an ensemble of random matrices corresponding to one of the classical compact groups equipped with Haar measure, i.e. one of the following groups: $\mathrm{U}(N)$, $\mathrm{Sp}(2N)$ and $\mathrm{O}^{\pm}(N)$, where the superscript $\pm$ indicates the connected component of the orthogonal group with determinant ± 1. From the point of view of the entanglement entropy (and of spin-spin correlations), quantum spin chains therefore divide into symmetry classes related to the classical compact groups. The XX model turns out to be an example of a system with $\mathrm{U}(N)$ symmetry. The averages that occur can be expressed either as Toeplitz determinants (i.e. determinants of matrices in which the elements are functions of the difference between the row and column indices), in the case of $\mathrm{U}(N)$, or as determinants of specific combinations of Toeplitz and Hankel matrices (i.e. matrices in which the elements are functions of the sum of the row and column indices) for the other compact groups. Asymptotic formulae for these determinants then lead to general expressions for the leading-order and next-to-leading-order terms in the asymptotics of the entanglement in the limit as the total number of spins tends to infinity and then as $N \to \infty$.

We find that at a critical point the entanglement grows logarithmically with N, in agreement with the conformal-field-theoretic calculations. We derive a general formula for the associated constant of proportionality. This is a rational number, the numerator of which is shown to

factorize into a universal part, related to symmetries of the quantum Hamiltonian and which can be calculated from the random-matrix averages, and a non-universal (i.e. Hamiltonian-specific) part, which we also evaluate. In the unitary case, comparing with the results in [5, 6, 9] leads to an explicit formula for the central charge. However, our approach also extends to systems where the conformal-field-theoretic results cannot be applied directly. These are the systems related to the other compact groups. Further details of our calculations and results may be found in [11].

The most general form of Hamiltonian related to quantum spin chains is

$$H_\alpha = \alpha \left[\sum_{j,k=0}^{M-1} b_j^\dagger A_{jk} b_k + \frac{\gamma}{2}\left(b_j^\dagger B_{jk} b_k^\dagger - b_j B_{jk} b_k \right) \right] - 2\sum_{j=0}^{M-1} b_j^\dagger b_j, \quad (2)$$

where α and γ are real parameters, $0 \le \gamma \le 1$, the b_js are Fermi oscillators, A is an Hermitian matrix, and B is an antisymmetric matrix. We take periodic boundary conditions, i.e. $b_M = b_0$. Without loss of generality, we will consider only matrices A and B with real elements. The Hamiltonian (2) can always be re-expressed in terms of the Pauli spin matrices using the Jordan-Wigner transformation [11, 12].

We will here be concerned with the entanglement between the first N oscillators and the rest of the chain when the system is in the ground state $|\mathbf{\Psi}_{\mathrm{g}}\rangle$ and as the length of chain tends to infinity. We decompose the Hilbert space into the direct product $\mathcal{H} = \mathcal{H}_{\mathrm{P}} \otimes \mathcal{H}_{\mathrm{Q}}$, where $\mathcal{H}_{\mathrm{P}}$ is generated by the first N sequential oscillators and $\mathcal{H}_{\mathrm{Q}}$ by the remaining $M-N$. Our goal is to determine the asymptotic behaviour for large $N << M$ of the von Neumann entropy $E_{\mathrm{P}} = -\operatorname{Tr}\rho_{\mathrm{P}}\log_2\rho_{\mathrm{P}}$, where $\rho_{\mathrm{P}} = \operatorname{Tr}_{\mathrm{Q}}\rho_{\mathrm{PQ}}$ and $\rho_{\mathrm{PQ}} = |\mathbf{\Psi}_{\mathrm{g}}\rangle\langle\mathbf{\Psi}_{\mathrm{g}}|$.

The first step involves determining the expectation values with respect to $|\mathbf{\Psi}_{\mathrm{g}}\rangle$ of products of arbitrary numbers of the operators

$$m_{2l+1} = \left(\prod_{j=0}^{l-1}\sigma_j^z\right)\sigma_l^x \quad \text{and} \quad m_{2l} = \left(\prod_{j=0}^{l-1}\sigma_j^z\right)\sigma_l^y. \quad (3)$$

From the invariance of the Hamiltonian (2) under the transformation $b_j \mapsto -b_j$, it follows that $\langle\mathbf{\Psi}_{\mathrm{g}}|\, m_l\, |\mathbf{\Psi}_{\mathrm{g}}\rangle = 0$; for the same reason, the expectation value of the product of an odd number of m_js must be zero. The expectation values $\langle\mathbf{\Psi}_{\mathrm{g}}|\, m_j m_k\, |\mathbf{\Psi}_{\mathrm{g}}\rangle$ can be deduced using the approach of Lieb *et al* [12]: $\langle\mathbf{\Psi}_{\mathrm{g}}|\, m_j m_k\, |\mathbf{\Psi}_{\mathrm{g}}\rangle = \delta_{jk} + \mathrm{i}(C_M)_{jk}$, where the correlation matrix C_M has the block structure

$$C_M = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1M} \\ C_{21} & C_{22} & \cdots & C_{2M} \\ \cdots & \cdots & \cdots & \cdots \\ C_{M1} & C_{M2} & \cdots & C_{MM} \end{pmatrix} \quad (4)$$

with

$$C_{jk} = \begin{pmatrix} 0 & (T_M)_{jk} \\ -(T_M)_{kj} & 0 \end{pmatrix}, \quad (5)$$

the matrix T_M is defined by

$$(T_M)_{jk} = \sum_{l=0}^{M-1} \psi_{lj}\phi_{lk}, \quad j,k = 0,\ldots,M-1, \quad (6)$$

and the vectors $\boldsymbol{\phi}_k$ and $\boldsymbol{\psi}_k$ are real and orthogonal and obey the eigenvalue equations

$$\alpha^2\left(A - \frac{2}{\alpha}I - \gamma B\right)\left(A - \frac{2}{\alpha}I + \gamma B\right)\boldsymbol{\phi}_k = |\Lambda_k|^2\boldsymbol{\phi}_k, \quad (7a)$$

$$\alpha^2\left(A - \frac{2}{\alpha}I + \gamma B\right)\left(A - \frac{2}{\alpha}I - \gamma B\right)\boldsymbol{\psi}_k = |\Lambda_k|^2\boldsymbol{\psi}_k. \quad (7b)$$

These vectors are related by

$$\alpha\left(A - \frac{2}{\alpha}I + \gamma B\right)\boldsymbol{\phi}_k = |\Lambda_k|\boldsymbol{\psi}_k, \quad (8a)$$

$$\alpha\left(A - \frac{2}{\alpha}I - \gamma B\right)\boldsymbol{\psi}_k = |\Lambda_k|\boldsymbol{\phi}_k. \quad (8b)$$

The expectation values of the product of an even number of m_js can then be computed using Wick's theorem (see, for example, [13]).

Following the calculation in [4], the formula for the entropy of the subchain P that one obtains using these expressions for the expectation values is then

$$E_{\mathrm{P}} = \lim_{\epsilon\to 0^+}\lim_{\delta\to 0^+}\frac{1}{2\pi\mathrm{i}}\oint_{c(\epsilon,\delta)} \mathrm{e}(1+\epsilon,\lambda)\frac{\mathrm{d}\ln D_N(\lambda)}{\mathrm{d}\lambda}\,\mathrm{d}\lambda, \quad (9)$$

where

$$\mathrm{e}(x,\nu) = -\frac{x+\nu}{2}\log_2\left(\frac{x+\nu}{2}\right) - \frac{x-\nu}{2}\log_2\left(\frac{x-\nu}{2}\right), \quad (10)$$

$D_N(\lambda) = \det(I\lambda - S)$, S is the real symmetric matrix $(T_N T_N^t)^{1/2}$ and T_N is obtained from the matrix (6) by removing the last $M-N$ rows and columns. The contour of integration $c(\epsilon,\delta)$ depends on the parameters ϵ and δ and includes the interval $[-1,1]$; as ϵ and δ tend to zero the contour approaches the interval $[-1,1]$. This guarantees that the branch points of $\mathrm{e}(1+\epsilon,\lambda)$ lie outside the contour of integration and thus that $\mathrm{e}(1+\epsilon,\lambda)$ is

analytic inside $c(\epsilon,\delta)$. The eigenvalues of S must all lie in the interval $[-1,1]$, and this is the case for the various Hamiltonians we consider [11].

We first specialize to cases where the Hamiltonian (2) is invariant under translations. For example, the XX model has this symmetry.

We denote $\overline{A}=\alpha A-2I$ and $\overline{B}=\alpha\gamma B$. If H_α is invariant under translations of the lattice $\{0,1,\ldots,M-1\}$, then the elements of the matrices $\overline{A}$ and $\overline{B}$ must depend only on the difference between the row and column indices, i.e. $\overline{A}$ and $\overline{B}$ must be Toeplitz matrices. In addition, because of the periodic boundary conditions, $\overline{A}$ and $\overline{B}$ must be *cyclic*.

Now, let a and b be two real functions on $\mathbb{Z}/M\mathbb{Z}$, even and odd respectively. The matrix elements of $\overline{A}$ and $\overline{B}$ can be written as

$$\overline{A}_{jk}=a(j-k)\quad\text{and}\quad\overline{B}_{jk}=b(j-k). \tag{11}$$

The complex exponentials

$$\phi_{kj}=\frac{\exp\left(\frac{2\pi\mathrm{i}kj}{M}\right)}{\sqrt{M}},\quad j,k=0,\ldots,M-1, \tag{12}$$

form a complete orthonormal set of eigenvectors of cyclic matrices, as can be easily verified by direct substitution. The matrices $\overline{A}$ and $\overline{B}$ defined in (11) commute. As a consequence, the complex exponentials (12) are a complete set of eigenvectors of $\overline{A}+\overline{B}$ too.

The eigenvalues of $\overline{A}+\overline{B}$ can be determined by inserting the eigenvectors (12) into the eigenvalue equations and using the parities of the functions $a(j)$ and $b(j)$. We have that when M is odd

$$\Lambda_k=a(0)+2\sum_{j=1}^{(M-1)/2}\left[a(j)\cos kj+\mathrm{i}b(j)\sin kj\right] \tag{13}$$

and when M is even

$$\begin{aligned}\Lambda_k&=a(0)+(-1)^l a(M/2)\\&\quad+2\sum_{j=1}^{M/2-1}\left[a(j)\cos kj+\mathrm{i}b(j)\sin kj\right],\end{aligned} \tag{14}$$

where $k=2\pi l/M$. Then

$$(T_N)_{jk}\xrightarrow[M\to\infty]{}\frac{1}{2\pi}\int_0^{2\pi}\frac{\Lambda(\theta)}{|\Lambda(\theta)|}\mathrm{e}^{-\mathrm{i}(j-k)\theta}\,\mathrm{d}\theta, \tag{15}$$

where $\Lambda(\theta)$ is the periodic function

$$\Lambda(\theta)=\sum_{j=-\infty}^{\infty}\Lambda_j\,\mathrm{e}^{\mathrm{i}j\theta} \tag{16}$$

with $\Lambda_j=a(j)-b(j)$ if $j>0$ and $\Lambda_j=a(j)+b(j)$ if $j<0$. Note that $T_N[g]$ is a Toeplitz matrix. $g(\theta)=\Lambda(\theta)/|\Lambda(\theta)|$ is called the symbol of T. It is worth emphasizing that (15) has been obtained by assuming only the translation invariance of the Hamiltonian (2) and periodic boundary conditions.

We now make the key observation that when $T_N[g]$ is symmetric the matrix S, which appears in the definition of $D_N(\lambda)$, is equal to T_N. We can then apply a famous identity of Heine [14] and Szegő [15], which asserts that if $G(U)$ is a function on $\mathrm{U}(N)$ that depends only on the eigenvalues $\exp(i\theta_j)$ of U and is such that $G(U)=\prod_{j=1}^N g(\theta_j)$, where $g(\theta)$ is 2π-periodic, then

$$\Big\langle G(U)\Big\rangle_{\mathrm{U}(N)}=\det\left(g_{j-k}\right)_{j,k=0,\ldots,N-1}, \tag{17}$$

where g_l is the lth Fourier coefficient of g. In our context, this implies that (9) can be expressed as an average with respect to Haar measure over the unitary group $\mathrm{U}(N)$, i.e. over the Circular Unitary Ensemble of $N\times N$ random matrices. A necessary and sufficient condition for $T_N[g]$ to be symmetric is that $\Lambda(\theta)$ should be real and even, or equivalently γ should be zero; in other words, the interaction in the Hamiltonian (2) must be isotropic. When $\gamma=0$ the symbol $g(\theta)$ is a piece-wise continuous function which takes the values 1 and -1 and has discontinuities at all points θ_r where the equation

$$\Lambda(\theta_r)=0 \tag{18}$$

is satisfied, with the additional condition that the first non-zero derivative of $\Lambda(\theta)$ at θ_r is odd.

Given that under the general conditions specified above the entropy of entanglement can be expressed as an average over $\mathrm{U}(N)$, it is natural to ask whether under different conditions it can be expressed as an average over random matrices drawn from the other classical groups. The question is: how are the symmetries of the Hamiltonian reflected in the group which determines the entropy of entanglement?

We begin with the orthogonal group $\mathrm{O}^+(2N)$. The analogue of the Heine-Szegő identity in this case relates group averages to the determinant of a sum of Toeplitz and Hankel matrices. A straightforward calculation generalizing that given above shows that this can be arranged for the spectral determinant D_N if (and only if) $\gamma=0$ and $\overline{A}_{jl}=a(j-l)+a(j+l)$ where, because of the periodic boundary conditions, a must be a function on $\mathbb{Z}/M\mathbb{Z}$ and must also be even in order for $\overline{A}$ to be symmetric. Note that the Hamiltonians in this class are not translation invariant. The properties of D_N are the same as those in the unitary case, except that $T_N[g]$ is the sum of a Toeplitz and a Hankel matrix. The symbol has the same general form as in the unitary case.

The calculations for the other compact groups follow exactly the same pattern except that for $\mathrm{Sp}(2N)$ and $\mathrm{O}^-(2N+2)$, $\overline{A}_{jk}=a(j-k)-a(j+k+2)$, and for $\mathrm{O}^\pm(2N+1)$, $\overline{A}_{jk}=a(j-k)\mp a(j+k+1)$. Again, in these cases the Hamiltonians are not translation invariant.

The asymptotics of the entropy of entanglement can now be calculated using the Fisher-Hartwig conjecture for the determinant D_N in the unitary case [16] and recent generalizations of this conjecture in the other cases [17, 18], and then by computing the integral in (9). The result is that as $N \to \infty$

$$E_{\mathrm{P}} \sim \frac{2^{w_{\mathrm{G}}} R}{6} \log_2 N, \tag{19}$$

where R is the number of solutions of (18) in the interval $[0, \pi)$ and

$$w_{\mathrm{G}} = \begin{cases} 1 & \text{if the average is over } \mathrm{U}(N) \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

The asymptotic relation (19) represents our main result. In the unitary case, comparing with the results of [5, 6, 9], it provides an explicit formula for the central charge, which may be seen to depend in a non-trivial way on the geometry of the Hamiltonian. In the case of the other classical compact groups, when the Hamiltonian is not translation invariant, the conformal-field-theoretic results do not apply directly. The factor $2^{w_{\mathrm{G}}}$ is universal, depending only on the symmetries determining the classical compact group to be averaged over. The factor R is Hamiltonian-dependent. For the XX model, which is an example with unitary symmetry, $R = 1$ and (19) coincides with the formula derived in [4].

Lower order terms in the Fisher-Hartwig conjecture and its generalizations lead directly to general formulae for the next-to-leading-order (constant) term $\tilde{\kappa}$ in the asymptotics of the entropy of entanglement when $N \to \infty$. For the unitary group we find

$$\tilde{\kappa}_{\mathrm{U}(N)} = \frac{R}{3 \ln 2} \left(K - 6 I_3 \ln 2 \right), \tag{21}$$

where I_3 is a constant evaluated in [4] to be $0.0221603\ldots$ and

$$K = 1 + \gamma_{\mathrm{E}} + \frac{1}{R} \sum_{r=1}^{R} \ln|1 - \mathrm{e}^{\mathrm{i}2\theta_r}| - \frac{2}{R} \sum_{1 \le r < s \le R} (-1)^{(r+s)} \ln \left| \frac{1 - \mathrm{e}^{\mathrm{i}(\theta_r - \theta_s)}}{1 - \mathrm{e}^{\mathrm{i}(\theta_r + \theta_s)}} \right|. \tag{22}$$

Here γ_{E} is Euler's constant. When $R = 1$ this equation reduces to the result of Jin and Korepin for the XX model. For the other compact groups we find, similarly, that $\tilde{\kappa} = \tilde{\kappa}_{\mathrm{U}(N)}/2 + R/6$.

We end with some general remarks. First, the circular ensembles of random matrices may be seen to play a special role in the context of the spin chains and boundary conditions we have considered here. It would be interesting to know whether the other random matrix ensembles may be used to describe systems with different interactions and boundary conditions. Second, we note that away from critical points $\Lambda(\theta)$ is continuous, and so $R = 0$, which is consistent with previous observations that the logarithmic growth of E_{P} is a critical phenomenon. Our approach determines the limiting value of E_{P} away from critical points too. Finally, the calculations and results described above extend straightforwardly to spin-spin correlations in the families of quantum spin chains we have considered.

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[1] C. H. Bennett, H. J. Bernstein, S. Popescu and B. Schumacher, *Phys. Rev. A*, **53** (1996), 2046.
[2] L. Amico, A. Osterloh, F. Plastina, R. Fazio and G. M. Palma, *Phys. Rev. A*, **69** (2004), 022304.
D. Aharonov, *Phys. Rev. A*, **62** (2000), 062311.
T. J. Osborne and M. A. Nielsen, *Phys. Rev. A*, **66** (2002), 032110.
A. Osterloh, L. Amico, G. Falci and R. Fazio, *Nature*, **416** (2002), 608.
[3] G. Vidal, J. I. Latorre, E. Rico and A. Kitaev, *Phys. Rev. Lett.*, **90** (2003), 227902.
[4] B. Q. Jin and V. E. Korepin, *J. Stat. Phys.*, **116** (2004), 79.
[5] V. E. Korepin, *Phys. Rev. Lett.*, **92** (2004), 096402.
[6] P. Calabrese and J. Cardy, *J. Stat. Mech.* P06002 (2004).
[7] N. Lambert, C. Emary and T. Brandes, *Phys. Rev. Lett.*, **92** (2004), 073602.
[8] F. Verstraete, M.A. Martin-Delgado and J. I. Cirac, *Phys. Rev. Lett.*, **92** (2004), 087201.
[9] C. Holzhey, F. Larsen and F. Wilczek, *Nucl. Phys.* B, **424** (1994), 443.
[10] The central charge of a conformal field theory may be defined (see, e.g., [5]) to be the limit as z tends to zero of $z^4 < T(z)T(0) >$, where $< T(z)T(0) >$ is the autocorrelation function of the zz-component of the energy-momentum tensor $T_{\mu,\nu}(z)$, z is the complex space-time variable $z = x + ivt$, and v is the Fermi velocity. Roughly speaking, the central charge counts the number of gapless degrees of freedom in the field theory.
[11] J. P. Keating and F. Mezzadri, *Commun. Math. Phys.*, **252** (2004), 543.
[12] E. Lieb, T. Schultz and D. Mattis, *Ann. Phys. (N.Y.)*, **16** (1961), 407.
[13] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Fields* (MacGraw-Hill, New York, 1965), p. 181
[14] E. Heine, *Handbuch der Kugelfunktionen* (G. Reimer, Berlin, 1878–81).
[15] G. Szegő. *Orthogonal Polynomials* (AMS, Providence, 1959)
[16] M. E. Fisher and R. E. Hartwig, *Adv. Chem. Phys.*, **15** (1968), 333.
[17] E. L. Basor and T. Ehrhardt, in *Toeplitz Matrices and Singular Integral Equations*, edited by A. Bottcher, I. Gohberg and P. Junghanns, [Op. Theory Adv. Appl. **135** (2002), 61]
[18] P. J. Forrester and N. E. Frankel, *J. Math. Phys. (N.Y.)*, **45** (2004), 2003.